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Phonon dispersion in hcp metals Cd, Sc and Y

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Phonon dispersion in hcp solids Cd, Sc and Y has been studied on the basis of a phenomenological model, earlier reported by us, which introduces a non-central interaction between nearest neighbours of different types arising from overlap of spheroidal ions The agreement between theory and experiments is found to be generally good

1. Introduction

A phenomenological model for the lattice dynamics of hcp metals (hereafter referred to as *I*) which introduces non central forces arising due to overlap ofspheroidal ions has recently been reported by Vibhute & Verma (1975 In this model the hexogonal symmetry about the c-axis suggests that the simplest shape the ion can have is a spheoid with the axis of revolution along the c-axis. The axial ratio of the spheroid can be chosen to be such as to lead to the observed axial ratio (c/a) of the solid on close packing. The overlap of these spheroidal ion leads to a force along the normal to the common tangent plane between the nearest neighbouring ions of different types. This normal deviation from the line of centres, the deviations being larger for larger deviations of the axial ratios (c/a) from the ideal value ($\sqrt{8/3} = 1\ 633$) obtained for the close packing of spheres. It is clear that the best test of the model can be those crystals which deviate from the ideal axial ratio by relatively large amounts. This is why this model has been applied to study the lattice dynamics of Zinc and berrylium with results which were as good as obtained by applying the modified axially symmetric mdel of de Wames *et al* (1965).

The model has successfully been applied to the study of other hcp metals also viz. Th and Zr. Cadmium is another hcp metal with a large c/a ratio. This solid poses severe difficulties to the determination of the phonon frequencies by the neutron scattering technique. However, the experimental phonon dispersion curves in this solid have been recently determined by the X-ray scattering-method by Toussaint & Champier (1972) who have interpreted their results using a six neighbour generalised tensor force model involving twenty two parameter and a pseudopotential model due to Ho (1968) In this communication we are presenting results on phonon dispersion of Cd obtained by the model described in I together with those on Sc and Y which have relatively simple electron configuration among the hcp solids and their c/a ratios deviate from the ideal values on the opposite direction of that in Cd It isobserved that our fifteen parameter

model gives better results on Cd than those obtained by the pseudopotential calculation of Ho and as good as those derived from the twenty two parameter tensor force model of Toussaint and Champier. Our results on other solids Sc and Y also present agreements with experimental dispersion curves which are as good as those obtained by a six neighour MAS model calculation of Wakabayashi *et al* (1971) and Sinha *et al* (1970) and better than those obtained by Upadhyay & Verma (1973) using a five neighbour central pair potential electron gas model.

We may mention here, however, that our model introduces non central interactions only between the nearest neighbouring atoms unlike the MAS and the interactions coupling the origin atom with the third to the sixth neighbours are entirely central. Further the non-central interaction introduced by us has a physical basis in the spheroidal shape of the ions This shape is not only dictated by the phenomenological considerations concerning the deviation of the c/a r-tio from the ideal value as explained above but may also be suggested by the electron density distributions around each ion calculated from the electron wave function For example LCAO approximations applied to the conduction electron wave function show that the d orbitals of A_{1g} type have a lobe along the c-axis and the E_{1g} and E_{2g} types have nodes in this direction. It is obvious that the electron densities calculated from such wave functions would give to the ion a shape which can better be approximated by a spheroid than as sphere.

2. Calculations and Results

The model used is that described in I and involves fifteen parameters Twelve of these parameters α_i, β_i ($i = 1$ to 6) are derived from the six neighbour central pair potentials and are related to the first and second derivatives of the pair potential. The parameters λ and μ arise from the overlap between spheroidal neighbours of different types and Ke is the bulk modulus of the electron gas We use the five elastic constants and nine zone centre and zone boundary frequencies to obtain fourteen of the fifteen parameters and the fifteenth is determined by varying it to obtain the best agreement with the experimental dispersion curves, simultaneously checking with the rotational invariance condition as explained in I. Sometined the solutions of these large number of simultaneous equations land into such values of model parameters which do not even approximately satisfy the rotational invariance condition. In all such cases, however a small variation ($\leqslant 5\%$) of one of the zone boundary frequencies viz. $\nu_{LO}(M)$ results into reasonably good set of values which approximately satisfy the rotational invariance condition It may be, therefore, expected that a least square fit programme could certainly improve the model parameters and hence the phonon frequencies significantly. This optimism is based on the fact that even a variation in one single frequency yields results which are generally in very good agreement with the corresponding experimental ones.

The input data for the three solids with relevant references are listed in Table 1 and the values of the model parameters in Table 2. The dispersion

Table 1. Input data for calculation of phonon frequencies

Constant	Cd	Sc	Y
a (Å)	2·973	3·309	3·6474
c (Å)	5 606	5 268	5 7306
m (amu)	112 41	44 956	88·919
c_{11}	1·158	0·993	0 779
c_{12}	0 3975	0 457	0 285
c_{33}	0 514	1·069	0·769
c_{44}	0·2039	0 277	0 2431
c_{13}	0 406	0 294	0·210
$\nu_{LO}(\Gamma)$	2·857	6·91	4 64
$\nu_{TO}(\Gamma)$	1·57	0·04	2·68
$\nu_{LA}(A)$	1 857	4·74	3·20
$\nu_{TA}''(M)$	2·35	3·57	2·30
$\nu_{TO}''(M)$	2·50	6·11	4·04
$\nu_{TA\perp}(M)$	1·28	3 97	2·67
$\nu_{TO\perp}(M)$	1 859	6·23	4 14
$\nu_{LA}(M)$	5·14	6·21	4 02
$\nu_{LO}(M)$	6·35	6·23	4 15

Table 2. Evaluated force parameters (in units of 10^4 dyn. cm^{-1}) and bulk modulus (Ke) (in 10^{12} dyn. cm^2)

Parameter	Cd	Sc	Y
K_e	+0·1514	+0·2393	+0·0755
μ	+5·5066	+3·0467	−0 1707
λ	+5·7750	−9·9511	−6·9159
β_1	+3·7061	+1·2081	+1·0539
β_2	+0 4040	+5·1849	+3·0688
β_3	−0·5272	+0·1150	+0·1965
β_4	−0·1745	−0·2958	−0·1415
β_5	+0·0436	−0·3686	−0·2174
β_6	−0·4790	+0 2576	+0·2158
α_1	−0·1396	+0 2253	+0·0996
α_2	−5·8053	−2·9681	+0·1206
α_3	+0·3927	−0·1858	−0·1940
α_4	+0·0258	−0·0508	−0·0168
α_5	+0·0530	+0·1593	+0·1218
α_6	0·0000	−0·1000	−0·1000

curves for Cd, Sc and Y derived from these parameters are shown in figures 1, 2 and 3 respectively together with experimental points and curves (shown dotted)

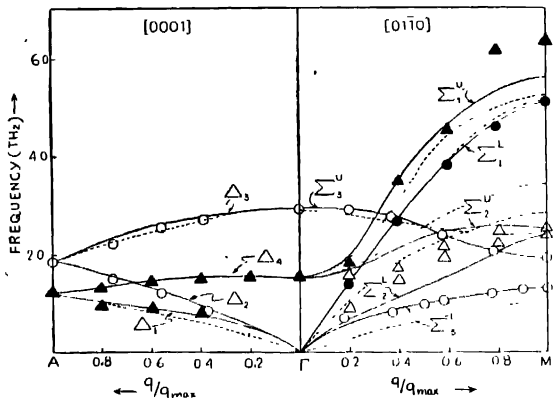

Fig. 1. Phonon dispersion curves of Cd.
●△▲O Experimental points.
—·—·— Theoretical-present study
– – – Theoretical pseudopotential model of Ho (1968)

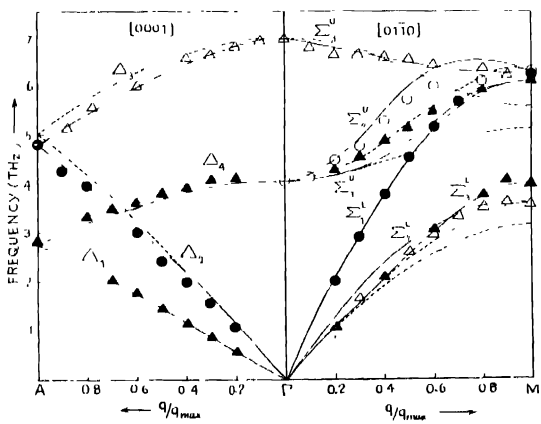

Fig. 2. Phonon dispersion curves of Sc
●△▲O Experimental points
—·—·— Theoretical-present study
– – – Theoretical (Upadhyaya & Serma (1973)

obtained in other theoretical studies. In figures 2 and 3 we have not shown the theoretical curves of Wakabayashi *et al* and Sinha *et al* as these curves mostly overlap with ours and present the same degree of agreement with the experimental curves. Generally speaking we find that the acoustic branches present a slightly

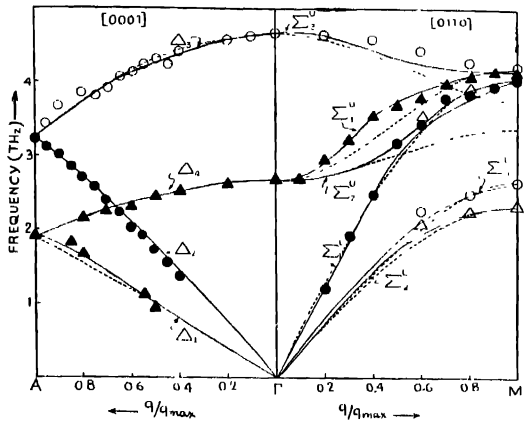

Fig. 3. Phonon dispersion curves of Y
●ΔAO Experimental points
——— Theoretical—present study
– – – Theoretical (Upadhyaya & Verma (1973).

better fit in our scheme and the optical ones are slightly better represented in the MAS scheme However, the agreement obtained by us in the result of direct calculations as against the least square fit obtained by these other authors. We have not resorted to the least squ have not resorted to the least square fit procedure just to avoid heavy computer bills but it can be expected that such a procedure will certainly lead to even better agreements than already obtained by us. Thus our 6 neighbour model which uses non-central interactions only between nearest two neighbours is at least as good as the six neighbour MAS mdoel The parameters λ and μ derived from the non-central interaction in our model are invariably large and this suggests that the origin of non-central interaction through the overlap of spheroidal ions may be a plausible assumption

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